

Time delay for dispersive systems in quantum scattering theory. I. The Friedrichs model

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Abstract

We present a method for proving the existence of time delay (defined in terms of sojourn times) as well as its identity with Eisenbud-Wigner time delay in the case of the Friedrichs model. We show that this method applies to scattering by finite rank potentials.

1 Introduction

One can find a large literature on the identity of Eisenbud-Wigner time delay and time delay in quantum scattering defined in terms of sojourn times (see [2, 6, 8, 12, 18, 19, 20, 25, 26, 27, 28, 29, 33, 34, 40] and references therein). However, most of the papers treat scattering processes where the free dynamics is given by a Schrödinger operator. The mathematical articles where different scattering processes are considered (such as [19, 25, 26, 33]) only furnish explicit applications in the Schrödinger case. The purpose of the present paper and the forthcoming work [38] is to fill in this gap by proving the existence of time delay and its identity with Eisenbud-Wigner time delay for a general class of dispersive quantum systems. Using a symmetrization argument introduced in [9, 26, 36] for N -body scattering, and rigorously applied in [4, 16, 24, 37, 39], we shall treat any two-body scattering process with free dynamics given by a regular enough pseudodifferential, or multiplication, operator. In this paper we restrict ourselves to the simple, but instructive, quantum model introduced by Friedrichs [15]. The general case will be considered elsewhere [38].

Let $H_0 := Q$ be the position operator in the Hilbert space $\mathcal{H} := L^2(\mathbb{R})$, endowed with the norm $\|\cdot\|$ and the scalar product $\langle \cdot, \cdot \rangle$. Let H be a selfadjoint perturbation of H_0 such that the wave operators $W_{\pm} := s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0}$ exist and are complete (so that the scattering operator $S := W_+^* W_-$ is unitary). Take a (localization) function

$f \in L^\infty(\mathbb{R}; \mathbb{C})$ decaying sufficiently fast at infinity. Then we define for some states $\varphi \in \mathcal{H}$ and $r > 0$ the quantities

$$\begin{aligned} T_r^0(\varphi) &:= \int_{\mathbb{R}} dt \langle e^{-itH_0} \varphi, f(P/r) e^{-itH_0} \varphi \rangle, \\ T_r(\varphi) &:= \int_{\mathbb{R}} dt \langle e^{-itH} W_- \varphi, f(P/r) e^{-itH} W_- \varphi \rangle, \\ \tau_r^{\text{in}}(\varphi) &:= T_r(\varphi) - T_r^0(\varphi), \\ \tau_r(\varphi) &:= T_r(\varphi) - \frac{1}{2} [T_r^0(\varphi) + T_r^0(S\varphi)], \end{aligned}$$

where P is the momentum operator in \mathcal{H} . If $\|\varphi\| = 1$ and f is the characteristic function χ_J for a bounded set $J \subset \mathbb{R}$, then these numbers admit a simple interpretation. The operator $f(P/r) \equiv \chi_{rJ}(P)$ is the orthogonal projection onto the set of states with momentum localised in $rJ := \{x \in \mathbb{R} \mid x/r \in J\}$. Therefore $T_r^0(\varphi)$ is the time spent by the freely evolving state $e^{-itH_0} \varphi$ in the subset $\chi_{rJ}(P)\mathcal{H}$ of \mathcal{H} (i.e. the time during which $e^{-itH_0} \varphi$ has momentum in rJ). Similarly $T_r(\varphi)$ is the time spent by the associated scattering state $e^{-itH} W_- \varphi$ in $\chi_{rJ}(P)\mathcal{H}$. Then $\tau_r^{\text{in}}(\varphi)$ is the time delay in $\chi_{rJ}(P)\mathcal{H}$ of the scattering process with incoming state φ , and $\tau_r(\varphi)$ is the corresponding symmetrized time delay. One can give an equivalent interpretation, with momenta replaced by positions, by using the Fourier transformation.

In this paper we study the existence of $\tau_r^{\text{in}}(\varphi)$ and $\tau_r(\varphi)$ as $r \rightarrow \infty$. Under general assumptions on f , H , and φ we show in Lemma 3.2.(b) that

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = \lim_{r \rightarrow \infty} \tau_r(\varphi)$$

whenever one of the two limits exists. In Theorem 3.4 and Remark 3.6 we prove the Eisenbud-Wigner formula for the Friedrichs model in an abstract setting. For general f , H , and φ , we show that

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = -i \int_{\mathbb{R}} dx |\varphi(x)|^2 \overline{S(x)} S'(x) \quad (1.1)$$

if the scattering matrix $x \mapsto S(x)$ is continuously differentiable on the support of φ . Some comments on the relation between Equation (1.1) and the Birman-Krein formula are given in Remark 3.7. In Section 4 we verify the assumptions of Theorem 3.4 and Remark 3.6 when H is a regular enough finite rank perturbation of H_0 . The main difficulty consists in showing (as in the Schrödinger case [3, 22]) that the scattering operator maps some dense set $\mathcal{E} \subset \mathcal{H}$ into itself. Essentially this reduces to proving that the scattering matrix is sufficiently differentiable on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$, which is achieved by proving a stationary formula for $S(x)$ and by using higher order commutators methods (see Lemmas 4.2-4.5). All these results are collected in Theorem 4.7, where Equation (1.1) is proved for finite rank perturbations. Some properties of a restriction operator [23, Chap. 2.4] are recalled in the appendix.

We emphasize that our approach relies crucially on the proof of the propagation formula

$$\lim_{r \rightarrow \infty} \int_0^\infty dt \langle \varphi, [e^{itH_0} f(P/r) e^{-itH_0} - e^{-itH_0} f(P/r) e^{itH_0}] \varphi \rangle = 2 \langle \varphi, P\varphi \rangle, \quad (1.2)$$

which relates the time evolution of the localization operator $f(P/r)$ to the energy derivative $iP \equiv \frac{d}{dH_0}$ (see Proposition 2.3). It allows us to establish Equation (1.1) for a general class of localization functions f not considered before (see Assumption (2.1)). In [38] we will generalise Equation (1.2) to the case of pseudodifferential operators H_0 .

We finally mention the paper [7] for a related work on sojourn time for the Friedrichs model.

2 Propagation formula for $H_0 = Q$

We give here the proof of Equation (1.2) under appropriate assumptions on the localization f and the vector φ .

Assumption 2.1. *The function $f \in L^\infty(\mathbb{R}; \mathbb{C})$ satisfies the following conditions:*

- (i) $f(x) = f(|x|)$ for a.e. $x \in \mathbb{R}$.
- (ii) There exists $\rho > 1$ such that $|f(x)| \leq \text{Const.} \langle x \rangle^{-\rho}$ for a.e. $x \in \mathbb{R}$.
- (iii) There exists $\delta > 0$ such that $f = 1$ on $(-\delta, \delta)$.

It is clear that $\text{s-lim}_{r \rightarrow \infty} f(P/r) = 1$ if f satisfies Assumption 2.1. The typical example of function f one should keep in mind is the following.

Example 2.2. *Let $f = \chi_J$, where $J \subset \mathbb{R}$ is bounded, symmetric (i.e. $J = -J$), and contains an interval $(-\delta, \delta)$ for some $\delta > 0$. Then f satisfies Assumption 2.1, and $f(P/r)$ is the orthogonal projection onto the set of states with momentum localised in rJ .*

For each $s, t \in \mathbb{R}$, we denote by \mathcal{H}_t^s the usual weighted Sobolev space over \mathbb{R} , i.e. the completion of the Schwartz space \mathcal{S} on \mathbb{R} for the norm $\|\varphi\|_{\mathcal{H}_t^s} := \| \langle P \rangle^s \langle Q \rangle^t \varphi \|$, $\langle \cdot \rangle := (1 + |\cdot|^2)^{1/2}$. We also set $\mathcal{H}^s := \mathcal{H}_0^s$ and $\mathcal{H}_t := \mathcal{H}_t^0$.

Proposition 2.3. *Let f satisfy Assumption 2.1. Then we have for each $\varphi \in \mathcal{H}^s$, $s > 1$,*

$$\lim_{r \rightarrow \infty} \int_0^\infty dt \langle \varphi, [e^{itQ} f(P/r) e^{-itQ} - e^{-itQ} f(P/r) e^{itQ}] \varphi \rangle = 2 \langle \varphi, P\varphi \rangle.$$

Proof. Let $r > 0$. Using the formula

$$e^{itQ} f(P/r) e^{-itQ} = f\left(\frac{P-t}{r}\right), \quad t \in \mathbb{R}, \quad (2.3)$$

one gets

$$\begin{aligned} I_r &:= \int_0^\infty dt \langle \varphi, [e^{itQ} f(P/r) e^{-itQ} - e^{-itQ} f(P/r) e^{itQ}] \varphi \rangle \\ &= \int_0^\infty dt \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 [f(\frac{k-t}{r}) - f(\frac{k+t}{r})], \end{aligned}$$

where \mathcal{F} stands for the Fourier transformation. Due to Assumption 2.1.(ii) one can apply Fubini's theorem to interchange the order of integration. This together with Assumption 2.1.(i) implies that

$$I_r = 2r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \operatorname{sgn}(k) \int_0^{|k|/r} dt f(t).$$

By Assumption 2.1.(iii) there exists $\delta > 0$ such that $f(t) = \chi_{[0,\delta)}(t) + \chi_{[\delta,\infty)}(t)f(t)$ for each $t \geq 0$. Thus $I_r = I_r^{(1)} + I_r^{(2)}$ with

$$I_r^{(1)} := 2r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \operatorname{sgn}(k) \int_0^{|k|/r} dt \chi_{[0,\delta)}(t),$$

and

$$I_r^{(2)} := 2r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \operatorname{sgn}(k) \int_0^{|k|/r} dt \chi_{[\delta,\infty)}(t)f(t).$$

Since $\varphi \in \mathcal{H}^s$ for some $s > 1$, one has

$$\begin{aligned} |I_r^{(2)}| &\leq \operatorname{Const.} r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \chi_{[\delta r, \infty)}(|k|) |k|/r \\ &\leq \operatorname{Const.} \|\langle P \rangle^{1/2} \chi_{[\delta r, \infty)}(|P|) \varphi\|^2 \\ &\leq \operatorname{Const.} \|\langle P \rangle^{1/2-s} \chi_{[\delta r, \infty)}(|P|)\|^2 \|\langle P \rangle^s \varphi\|^2 \\ &\leq \operatorname{Const.} \langle \delta r \rangle^{1-2s}. \end{aligned} \tag{2.4}$$

Thus $\lim_{r \rightarrow \infty} I_r = \lim_{r \rightarrow \infty} I_r^{(1)}$. Since

$$\int_0^{|k|/r} dt \chi_{[0,\delta)}(t) = \delta \chi_{[\delta r, \infty)}(|k|) + \frac{|k|}{r} \chi_{[0, \delta r)}(|k|),$$

one has

$$I_r^{(1)} = 2\delta r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \operatorname{sgn}(k) \chi_{[\delta r, \infty)}(|k|) + 2 \int_{\mathbb{R}} dk k |(\mathcal{F}\varphi)(k)|^2 \chi_{[0, \delta r)}(|k|).$$

But calculations similar to (2.4) show that

$$|2\delta r \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 \operatorname{sgn}(k) \chi_{[\delta r, \infty)}(|k|)| \leq \operatorname{Const.} r^{1-s}.$$

It follows that

$$\lim_{r \rightarrow \infty} I_r = \lim_{r \rightarrow \infty} I_r^{(1)} = \lim_{r \rightarrow \infty} 2 \int_{\mathbb{R}} dk k |(\mathcal{F}\varphi)(k)|^2 \chi_{[0, \delta r)}(|k|) = 2 \langle \varphi, P \varphi \rangle,$$

which proves the claim. \square

3 Time delay

In this section we prove the existence of time delay for the Friedrichs model in \mathcal{H} with free Hamiltonian $H_0 = Q$ and full Hamiltonian H . The full Hamiltonian H can be any selfadjoint operator in \mathcal{H} satisfying the following condition (we write $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ for the set of bounded operators from a Hilbert space \mathcal{H}_1 to a Hilbert space \mathcal{H}_2).

Assumption 3.1. *The wave operators W_{\pm} exist and are complete, and any operator $T \in \mathcal{B}(\mathcal{H}^{-s}, \mathcal{H})$, with $s > 1/2$, is locally H -smooth on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$.*

For each $s \geq 0$ we introduce the set

$$\mathcal{D}_s := \{\varphi \in \mathcal{H}^s \mid \chi_J(Q)\varphi = \varphi \text{ for some compact set } J \subset \mathbb{R} \setminus \sigma_{\text{pp}}(H)\}.$$

It is clear that \mathcal{D}_s is dense in \mathcal{H} if $\sigma_{\text{pp}}(H)$ is of Lebesgue measure 0 and that $\mathcal{D}_{s_1} \subset \mathcal{D}_{s_2}$ if $s_1 \geq s_2$. Furthermore if $\varphi \in \mathcal{D}_0$, then $T_r(\varphi)$ is finite for each $r > 0$ due to Assumption 3.1.

For each $r > 0$, we define

$$\begin{aligned} \tau_r^{\text{free}}(\varphi) &:= \frac{1}{2} \int_0^\infty dt \langle S\varphi, [e^{itH_0} f(P/r) e^{-itH_0} - e^{-itH_0} f(P/r) e^{itH_0}] S\varphi \rangle \\ &\quad - \frac{1}{2} \int_0^\infty dt \langle \varphi, [e^{itH_0} f(P/r) e^{-itH_0} - e^{-itH_0} f(P/r) e^{itH_0}] \varphi \rangle. \end{aligned} \quad (3.5)$$

The number $\tau_r^{\text{free}}(\varphi)$ (which has the dimension of a time if $f(P/r)$ is an orthogonal projection) is finite for all $\varphi \in \mathcal{H}$. We refer the reader to [4, Eq. (93) & (96)], [16, Eq. (4.1)], and [39, Sec. 2.1] for similar definitions when H_0 is the free Schrödinger operator and $f(P/r)$ is an orthogonal projection. The usual definition can be found in [2, Eq. (3)], [20, Eq. (6.2)], and [25, Eq. (5)].

Lemma 3.2. *Let f satisfy Assumption 2.1 and suppose that Assumption 3.1 holds. Then*

(a) *For each $r > 0$ and $\varphi \in \mathcal{H}$ one has the identities*

$$T_r^0(\varphi) = r\|\varphi\|^2 \int_{\mathbb{R}} dx f(x), \quad T_r^0(\varphi) = T_r^0(S\varphi), \quad \tau_r^{\text{in}}(\varphi) = \tau_r(\varphi). \quad (3.6)$$

(b) *Suppose that $f \geq 0$ and let $\varphi \in \mathcal{D}_0$ be such that*

$$\|(W_- - 1) e^{-itH_0} \varphi\| \in L^1(\mathbb{R}_-, dt) \quad (3.7)$$

and

$$\|(W_+ - 1) e^{-itH_0} S\varphi\| \in L^1(\mathbb{R}_+, dt). \quad (3.8)$$

Then

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = \lim_{r \rightarrow \infty} \tau_r(\varphi) = \lim_{r \rightarrow \infty} \tau_r^{\text{free}}(\varphi).$$

Proof. (a) Formula (2.3) and Assumption 2.1.(i) give

$$T_r^0(\varphi) = \int_{\mathbb{R}} dt \int_{\mathbb{R}} dk |(\mathcal{F}\varphi)(k)|^2 f\left(\frac{t-k}{r}\right).$$

Then Fubini's theorem (which is applicable due to Assumption 2.1.(ii)) and the change of variable $x := \frac{t-k}{r}$ imply the first identity in (3.6). The remaining identities follow from the first identity.

(b) The first equality follows from the third identity in point (a). Since $f \geq 0$ one has

$$\begin{aligned} \tau_r(\varphi) - \tau_r^{\text{free}}(\varphi) &= \int_0^\infty dt \left[\left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH} W_- \varphi \right\|^2 - \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH_0} S \varphi \right\|^2 \right] \\ &\quad + \int_{-\infty}^0 dt \left[\left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH} W_- \varphi \right\|^2 - \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH_0} \varphi \right\|^2 \right]. \end{aligned} \quad (3.9)$$

Using the inequality

$$|\|u\|^2 - \|v\|^2| \leq \|u - v\| (\|u\| + \|v\|), \quad u, v \in \mathcal{H},$$

and the completeness of W_\pm , we obtain the estimates

$$\left| \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH} W_- \varphi \right\|^2 - \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH_0} \varphi \right\|^2 \right| \leq \text{Const. } f_-(t) \|\varphi\| \quad (3.10)$$

$$\left| \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH} W_- \varphi \right\|^2 - \left\| f\left(\frac{P}{r}\right)^{1/2} e^{-itH_0} S \varphi \right\|^2 \right| \leq \text{Const. } f_+(t) \|\varphi\|, \quad (3.11)$$

where

$$f_-(t) := \|(W_- - 1) e^{-itH_0} \varphi\| \quad \text{and} \quad f_+(t) := \|(W_+ - 1) e^{-itH_0} S \varphi\|.$$

We know from Hypotheses (3.7)-(3.8) that $f_\pm \in L^1(\mathbb{R}_\pm, dt)$. Furthermore since $s\text{-}\lim_{r \rightarrow \infty} f(\frac{P}{r})^{1/2} = 1$, the scalars on the l.h.s. of (3.10)-(3.11) converge to 0 as $r \rightarrow \infty$. Therefore the claim follows from (3.9) and Lebesgue's dominated convergence theorem. \square

Remark 3.3. The “velocity” operator associated to the free evolution group e^{itQ} is constant due to the canonical commutation rule, namely

$$\frac{d}{dt} (e^{itQ} P e^{-itQ}) = -1.$$

Therefore the propagation speed of a state $e^{itQ} \varphi$ in the space of momenta is equal to -1 . In that respect the identities of Lemma 3.2.(a) are natural. For example, if $\|\varphi\| = 1$ and $f = \chi_J$ is as in Example 2.2, then $T_r^0(\varphi) = r|J|$, where $|J|$ is the Lebesgue measure of J . In such a case $T_r^0(\varphi)$ is nothing else but the sojourn time in rJ (in the space of momenta) of the state $e^{itQ} \varphi$ propagating at speed -1 .

Next Theorem is a direct consequence of Formula (3.5), Proposition 2.3, and Lemma 3.2.(b).

Theorem 3.4. *Let $f \geq 0$ satisfy Assumption 2.1. Suppose that Assumption 3.1 holds. For some $s > 1$, let $\varphi \in \mathcal{D}_s$ satisfy (3.7)-(3.8) and $S\varphi \in \mathcal{D}_s$. Then*

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = \langle \varphi, S^*[P, S]\varphi \rangle. \quad (3.12)$$

Remark 3.5. *Formula (3.12) shows that $\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi)$ is null if the commutator $[P, S]$ vanishes (which happens if and only if the scattering operator S is constant). We give an example of Hamiltonian H for which this occurs.*

Let $\widetilde{H}_0 := P$ with domain $\mathcal{D}(\widetilde{H}_0) := \mathcal{H}^1$, and for $q \in \mathcal{H}$ let $\widetilde{H} := \widetilde{H}_0 + q(Q)$ with domain $\mathcal{D}(\widetilde{H}) := \{\varphi \in \mathcal{H}^1 \mid \widetilde{H}\varphi \in \mathcal{H}\}$. It is known [42, Sec. 2.4.3] that \widetilde{H} is selfadjoint, that the wave operators $\widetilde{W}_{\pm} := \text{s-lim}_{s \rightarrow \pm\infty} e^{it\widetilde{H}} e^{-it\widetilde{H}_0}$ exist and are complete, and that $\widetilde{S} := \widetilde{W}_+^ \widetilde{W}_- = e^{-i \int_{\mathbb{R}} dx q(x)}$ is constant. Therefore $H := \mathcal{F}\widetilde{H}\mathcal{F}^{-1} = H_0 + q(-P)$ is selfadjoint on $\mathcal{D}(H) := \mathcal{F}\mathcal{D}(\widetilde{H})$, the wave operators $W_{\pm} = \mathcal{F}\widetilde{W}_{\pm}\mathcal{F}^{-1}$ exist and are complete, and $S = \widetilde{S}$.*

Remark 3.6. *Suppose that the assumptions of Theorem 3.4 are verified, and for a.e. $x \in \mathbb{R}$ let $S(x) \in \mathbb{C}$ be the component at energy x of the scattering matrix associated to the scattering operator S . Then Equation (3.12) can be rewritten as*

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = -i \int_{\mathbb{R}} dx |\varphi(x)|^2 \overline{S(x)} S'(x) \quad (3.13)$$

if the function $x \mapsto S(x)$ is continuously differentiable on the support of φ (note that Equation (3.13) does not follow from [25] or [5, Chap. 7.2], since we do not require $f(P/r)$ to be an orthogonal projection or $x \mapsto S(x)$ to be twice differentiable on the whole real line). Formula (3.13) holds for the general class of functions $f \geq 0$ satisfying Assumption 2.1. However, if $\|\varphi\| = 1$ and $f = \chi_J$ is as in Example 2.2, then we know that the scalars $T_r^0(\varphi)$ and $T_r(\varphi)$ can be interpreted as sojourn times. Therefore in such a case Formula (3.13) expresses the identity of the global time delay and the Eisenbud-Wigner time delay for the Friedrichs model.

Remark 3.7. *Let $R_0(\cdot)$ and $R(\cdot)$ be the resolvent families of H_0 and H , and suppose that $R(i) - R_0(i)$ is trace class. Then, at least formally, we get from the Birman-Krein formula [42, Thm. 8.7.2] that*

$$\overline{S(x)} S'(x) = -2\pi i \xi'(x; H, H_0), \quad (3.14)$$

where $\xi'(x; H, H_0)$ is the derivative of the spectral shift function for the pair $\{H_0, H\}$. Therefore one has

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = -2\pi \int_{\mathbb{R}} dx |\varphi(x)|^2 \xi'(x; H, H_0), \quad (3.15)$$

and the number $-2\pi\xi'(x; H, H_0)$ may be interpreted as the component at energy x of the time delay operator for the Friedrichs model. However Equations (3.14)-(3.15) turn out to be difficult to prove rigorously under this form. We refer to [19], [26, Sec. III.b], and [33, Sec. 3] for general theories on this issue, and to [11, 30, 41] for related works in the case of the Friedrichs-Faddeev model.

4 Finite rank perturbation

Here we apply the theory of Section 3 to finite rank perturbations of $H_0 = Q$. Given $u, v \in \mathcal{H}$ we write $P_{u,v}$ for the rank one operator $P_{u,v} := \langle u, \cdot \rangle v$, and we set $P_v := P_{v,v}$. The full Hamiltonian we consider is defined as follows.

Assumption 4.1. *Fix an integer $N \geq 0$ and take $\mu \geq 0$. For $j, k \in \{1, \dots, N\}$, let $v_j \in \mathcal{H}^\mu$ satisfy $\langle v_j, v_k \rangle = \delta_{jk}$, and let $\lambda_j \in \mathbb{R}$. Then $H := H_0 + V$, where $V := \sum_{j=1}^N \lambda_j P_{v_j}$.*

Many functions v_j (as the Hermite functions [32, p. 142]) satisfy the requirements of Assumption 4.1. Under Assumption 4.1 the perturbation V is bounded from $\mathcal{H}^{-\mu}$ to \mathcal{H}^μ , H is selfadjoint on $\mathcal{D}(H) = \mathcal{D}(H_0)$, and the wave operators W_\pm exist and are complete [31, Thm. XI.8].

In the next lemma we establish some of the spectral properties of H , we prove a limiting absorption principle for H , and we give a class of locally H -smooth operators. The limiting absorption principle is expressed in terms of the Besov space $\mathcal{K} := (\mathcal{H}^1, \mathcal{H})_{1/2,1} \equiv \mathcal{H}^{1/2,1}$ defined by real interpolation [1, Chap. 2]. We recall that for each $s > 1/2$ we have the continuous embeddings [10, p. 11]

$$\mathcal{H}^s \subset \mathcal{K} \subset \mathcal{H} \subset \mathcal{K}^* \subset \mathcal{H}^{-s}.$$

We refer the reader to [1, Sec. 6.2.1] for the definition of the regularity classes $C^k(A)$ and to [1, Sec. 7.2.2] for the definition of a (strict) Mourre estimate. The symbol \mathbb{C}_\pm stands for the half-plane $\mathbb{C}_\pm := \{z \in \mathbb{C} \mid \pm \operatorname{Im}(z) > 0\}$.

Lemma 4.2. *Let H satisfy Assumption 4.1 with $\mu \geq 2$. Then*

- (a) *H has at most a finite number of eigenvalues, and each of these eigenvalues is of finite multiplicity.*
- (b) *The map $z \mapsto (H - z)^{-1} \in \mathcal{B}(\mathcal{K}, \mathcal{K}^*)$, which is holomorphic on \mathbb{C}_\pm , extends to a weak* continuous function on $\mathbb{C}_\pm \cup \{\mathbb{R} \setminus \sigma_{\text{pp}}(H)\}$. In particular, H has no singularly continuous spectrum.*
- (c) *If T belongs to $\mathcal{B}(\mathcal{H}^{-s}, \mathcal{H})$ for some $s > 1/2$, then T is locally H -smooth on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$.*

The spectral results of points (a) and (b) on the finiteness of the singular spectrum of H are not surprising; they are known in the more general setting where V is an integral operator with Hölder continuous kernel (see e.g. [13, Thm. 1] and [14, Lemma 3.10]). Note however that point (a) implies that the sets \mathcal{D}_s are dense in \mathcal{H} for each $s \geq 0$.

Proof. (a) Let $A := -P$, then $e^{-itA} H_0 e^{itA} = H_0 + t$ for each $t \in \mathbb{R}$. Thus H_0 is of class $C^\infty(A)$ and satisfies a strict Mourre estimate on \mathbb{R} [1, Sec. 7.6.1]. Furthermore the quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \langle A\varphi, iV\varphi \rangle - \langle \varphi, iVA\varphi \rangle$$

extends uniquely to the bounded form defined by the rank $2N$ operator $F_1 := -\sum_{j=1}^N \lambda_j (P_{v_j, v'_j} + P_{v'_j, v_j})$. This means that V is of class $C^1(A)$. Thus H is of class $C^1(A)$ and since F_1 is compact, H satisfies a Mourre estimate on \mathbb{R} . The claim then follows by [1, Cor. 7.2.11].

(b) The quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \langle A\varphi, iF_1\varphi \rangle - \langle \varphi, iF_1A\varphi \rangle$$

extends uniquely to the bounded form defined by the rank $3N$ operator $F_2 := \sum_{j=1}^N \lambda_j (P_{v''_j, v_j} + 2P_{v'_j, v''_j} + P_{v_j, v''_j})$. This, together with [1, Thm. 7.2.9 & Thm. 7.2.13] and the proof of point (a), implies that H is of class $C^2(A)$ and that H satisfies a strict Mourre estimate on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$. It follows by [35, Thm. 01] (which applies to operators without spectral gap) that the map $z \mapsto (H - z)^{-1} \in \mathcal{B}(\mathcal{K}, \mathcal{K}^*)$ extends to a weak* continuous function on $\mathbb{C}_\pm \cup \{\mathbb{R} \setminus \sigma_{\text{pp}}(H)\}$. In particular, H has no singularly continuous spectrum in $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$. Since continuous Borel measures on \mathbb{R} have no pure points [32, p. 22] and since $\sigma_{\text{pp}}(H)$ is finite by point (a), we even get that H has no singularly continuous spectrum at all.

(c) Since T belongs to $\mathcal{B}(\mathcal{D}(H), \mathcal{H})$ and $T^*\mathcal{H} \subset \mathcal{H}^s \subset \mathcal{K}$, the claim is a consequence of [1, Prop. 7.1.3.(b)] and the discussion that follows. \square

We now study the differentiability of the function $x \mapsto S(x)$, which relies on the differentiability of the boundary values of the resolvent of H .

Lemma 4.3. *Let H satisfy Assumption 4.1 with $\mu \geq n + 1$ for some integer $n \geq 1$. Let $I \subset \{\mathbb{R} \setminus \sigma_{\text{pp}}(H)\}$ be a relatively compact interval, and take $s > n - 1/2$. Then for each $x \in I$ the limits*

$$R^n(x \pm i0) := \lim_{\varepsilon \searrow 0} (H - x \mp i\varepsilon)^{-n}$$

exist in the norm topology of $\mathcal{B}(\mathcal{H}^s, \mathcal{H}^{-s})$ and are Hölder continuous. Furthermore $x \mapsto R(x \pm i0)$ is $n - 1$ times (Hölder continuously) differentiable as a map from I to $\mathcal{B}(\mathcal{H}^s, \mathcal{H}^{-s})$, and

$$\frac{d^{n-1}}{dx^{n-1}} R(x \pm i0) = (n - 1)! R^n(x \pm i0).$$

Proof. The claims follow from [21, Thm. 2.2.(iii)] applied to our situation. We only have to verify the hypotheses of that theorem, namely that H is n -smooth with respect to $A = -P$ in the sense of [21, Def. 2.1]. This is done in points (a), (b), (c_n), (d_n), and (e) that follow.

(a) $\mathcal{D}(A) \cap \mathcal{D}(H) \supset \mathcal{S}$ is dense in $\mathcal{D}(H)$.

(b) Let $\varphi \in \mathcal{H}_1$ and $\theta \in \mathbb{R}$. Then one has

$$\|e^{i\theta A} \varphi\|_{\mathcal{H}_1} = \|\langle Q + \theta \rangle \varphi\| \leq \|\langle Q + \theta \rangle \langle Q \rangle^{-1}\| \cdot \|\varphi\|_{\mathcal{H}_1} \leq 2^{-1/2} (2 + |\theta|)^{1/2} \|\varphi\|_{\mathcal{H}_1}.$$

In particular, $e^{i\theta A}$ maps $\mathcal{D}(H)$ into $\mathcal{D}(H)$, and $\sup_{|\theta| \leq 1} \|H e^{i\theta A} \varphi\| < \infty$ for each $\varphi \in \mathcal{D}(H)$.

(c_n)-(d_n) Due to the proof Lemma 4.2.(a) the quadratic form

$$\mathcal{D}(A) \cap \mathcal{D}(H) \ni \varphi \mapsto \langle A\varphi, iH\varphi \rangle - \langle H\varphi, iA\varphi \rangle$$

extends uniquely to the bounded form defined by the operator $iB_1 := 1 + F_1$, where $F_1 = -\sum_{j=1}^N \lambda_j (P_{v'_j, v_j} + P_{v_j, v'_j})$. Similarly for $j = 2, 3, \dots, n+1$ the quadratic form

$$\mathcal{D}(A) \cap \mathcal{D}(H) \ni \varphi \mapsto \langle A\varphi, i(iB_{j-1})\varphi \rangle - \langle (iB_{j-1})^* \varphi, iA\varphi \rangle$$

extends uniquely to a bounded form defined by an operator $iB_j := F_j$, where F_j is a linear combination of the rank one operators $P_{v^{(j-k)}, v^{(k)}}$, $k = 0, 1, \dots, j$.

(e) Due to the proof Lemma 4.2.(a), H satisfies a Mourre estimate on \mathbb{R} . \square

For $m = 1, 2, \dots, N$ let $V_m := \sum_{j=1}^m \lambda_j P_{v_j}$ and $H_m := H_0 + V_m$. Then it is known that the scattering matrix $S(x)$ factorizes for a.e. $x \in \mathbb{R}$ as [42, Eq. (8.4.2)]

$$S(x) = \widetilde{S}_N(x) \cdots \widetilde{S}_2(x) \widetilde{S}_1(x), \quad (4.16)$$

where $\widetilde{S}_m(x)$ is unitarily equivalent to the scattering matrix $S_m(x)$ associated to the pair $\{H_m, H_{m-1}\}$. Since the difference $H_m - H_{m-1}$ is of rank one, one can even obtain an explicit expression for $S_m(x)$ (see [42, Eq. (6.7.9)]). For instance one has the following simple formula for $S_1(x)$ [42, Eq. (8.4.1)], [17, Eq. (66a)]

$$S_1(x) = \frac{1 + \lambda_1 F(x - i0)}{1 + \lambda_1 F(x + i0)},$$

where

$$F(x \pm i0) := \lim_{\varepsilon \searrow 0} \langle v_1, (H_0 - x \mp i\varepsilon)^{-1} v_1 \rangle.$$

Clearly Formula (4.16) is not very convenient for studying the differentiability of the function $x \mapsto S(x)$. This is why we prove the usual formula for $S(x)$ in the next lemma.

Given $\tau \in \mathbb{R}$, we let $\gamma(\tau) : \mathcal{S} \rightarrow \mathbb{C}$ be the restriction operator defined by $\gamma(\tau)\varphi := \varphi(\tau)$. Some of the regularity properties of $\gamma(\tau)$ are collected in the appendix. Here we only recall that $\gamma(\tau)$ extends uniquely to an element of $\mathcal{B}(\mathcal{H}^s, \mathbb{C})$ for each $s > 1/2$.

Lemma 4.4. *Let H satisfy Assumption 4.1 with $\mu \geq 2$. Then for each $x \in \mathbb{R} \setminus \sigma_{\text{pp}}(H)$ one has the equality*

$$S(x) = 1 - 2\pi i \gamma(x) [1 - VR(x + i0)] V \gamma(x)^*. \quad (4.17)$$

Proof. The claim is a consequence of the stationary method for trace class perturbations [42, Thm. 7.6.4] applied to the pair $\{H_0, H\}$.

The perturbation V can be written as a product $V = G^* G_0$, with $G := \sum_{j=1}^N \lambda_j P_{v_j}$ and $G_0 := \sum_{j=1}^N P_{v_j}$. Since the operators G and G_0 are selfadjoint and belong to the

Hilbert-Schmidt class, all the hypotheses of [42, Thm. 7.6.4] (and thus of [42, Thm. 5.7.1]) are trivially satisfied. Therefore one has for a.e. $x \in \mathbb{R}$ the equality

$$S(x) = 1 - 2\pi i \gamma(x) G [1 - \tilde{B}(x + i0)] G_0 \gamma(x)^*, \quad (4.18)$$

where $\tilde{B}(x + i0)$ is the norm limit defined by the condition

$$\lim_{\varepsilon \searrow 0} \|G_0(H - x - i\varepsilon)^{-1}G - \tilde{B}(x + i0)\| = 0.$$

On another hand we know from Lemma 4.3 that the limit $R(x + i0)$ exists in the norm topology of $\mathcal{B}(\mathcal{H}^s, \mathcal{H}^{-s})$ for each $x \in \mathbb{R} \setminus \sigma_{\text{pp}}(H)$ and each $s > 1/2$. Since we also have $G_0, G \in \mathcal{B}(\mathcal{H}^{-\mu}, \mathcal{H}^{\mu})$, we get the identity $\tilde{B}(x + i0) = G_0 R(x + i0) G$. This together with Formula (4.18) implies the claim. \square

We are in a position to show the differentiability of the scattering matrix.

Lemma 4.5. *Let H satisfy Assumption 4.1 with $\mu \geq n + 1$ for some integer $n \geq 1$. Then $x \mapsto S(x)$ is $n - 1$ times (Hölder continuously) differentiable from $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$ to \mathbb{C} .*

Proof. Due to Formula (4.17) it is sufficient to prove that the terms

$$A(x) := \left(\frac{d^{\ell_1}}{dx^{\ell_1}} \gamma(x)\right) V \left(\frac{d^{\ell_2}}{dx^{\ell_2}} \gamma(x)^*\right)$$

and

$$B(x) := \left(\frac{d^{\ell_1}}{dx^{\ell_1}} \gamma(x)\right) V \left(\frac{d^{\ell_2}}{dx^{\ell_2}} R(x + i0)\right) V \left(\frac{d^{\ell_3}}{dx^{\ell_3}} \gamma(x)^*\right)$$

exist and are locally Hölder continuous on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$ for all non-negative integers ℓ_1, ℓ_2, ℓ_3 satisfying $\ell_1 + \ell_2 + \ell_3 \leq n - 1$. The factors in $B(x)$ satisfy

$$\begin{aligned} \left(\frac{d^{\ell_3}}{dx^{\ell_3}} \gamma(x)^*\right) &\in \mathcal{B}(\mathbb{C}, \mathcal{H}^{-s_3}) \quad \text{for } s_3 > \ell_3 + 1/2, \\ V &\in \mathcal{B}(\mathcal{H}^{-s_3}, \mathcal{H}^{s_2}) \quad \text{for } s_2, s_3 \in [0, \mu], \\ \left(\frac{d^{\ell_2}}{dx^{\ell_2}} R(x + i0)\right) &\in \mathcal{B}(\mathcal{H}^{s_2}, \mathcal{H}^{-s_2}) \quad \text{for } s_2 > \ell_2 + 1/2, \\ V &\in \mathcal{B}(\mathcal{H}^{-s_2}, \mathcal{H}^{s_1}) \quad \text{for } s_1, s_2 \in [0, \mu], \\ \left(\frac{d^{\ell_1}}{dx^{\ell_1}} \gamma(x)\right) &\in \mathcal{B}(\mathcal{H}^{s_1}, \mathbb{C}) \quad \text{for } s_1 > \ell_1 + 1/2, \end{aligned}$$

and are locally Hölder continuous due to Lemma 4.3 and Lemma 4.8. Therefore if the s_j 's above are chosen so that $s_j \in (\ell_j + 1/2, \mu]$ for $j = 1, 2, 3$, then $B(x)$ is finite and locally Hölder continuous on $\mathbb{R} \setminus \sigma_{\text{pp}}(H)$. Since similar arguments apply to the term $A(x)$, the claim is proved. \square

Lemma 4.6. *Let H satisfy Assumption 4.1 with $\mu > 2$. Then one has for each $\varphi \in \mathcal{D}_s$, $s > 2$,*

$$\|(W_- - 1) e^{-itH_0} \varphi\| \in L^1(\mathbb{R}_-, dt) \quad (4.19)$$

and

$$\|(W_+ - 1) e^{-itH_0} \varphi\| \in L^1(\mathbb{R}_+, dt). \quad (4.20)$$

Proof. For $\varphi \in \mathcal{D}_s$ and $t \in \mathbb{R}$, we have (see *e.g.* the proof of [20, Lemma 4.6])

$$(W_- - 1) e^{-itH_0} \varphi = -i e^{-itH} \int_{-\infty}^t d\tau e^{i\tau H} V e^{-i\tau H_0} \varphi,$$

where the integral is strongly convergent. Hence to prove (4.19) it is enough to show that

$$\int_{-\infty}^{-\delta} dt \int_{-\infty}^t d\tau \|V e^{-i\tau H_0} \varphi\| < \infty \quad (4.21)$$

for some $\delta > 0$. Let $\zeta := \min\{\mu, s\}$, then $\|\langle P \rangle^\zeta \varphi\|$ and $\|V \langle P \rangle^\zeta\|$ are finite by hypothesis. If $|\tau|$ is big enough, it follows that

$$\begin{aligned} \|V e^{-i\tau H_0} \varphi\| &\leq \text{Const.} \|\langle P \rangle^{-\zeta} e^{-i\tau Q} \langle P \rangle^{-\zeta}\| = \text{Const.} \|\langle P - \tau \rangle^{-\zeta} \langle P \rangle^{-\zeta}\| \\ &\leq \text{Const.} |\tau|^{-\zeta}. \end{aligned}$$

Since $\zeta > 2$, this implies (4.21), and thus (4.19). The proof of (4.20) is similar. \square

In the next theorem we prove the existence of time delay and its identity with Eisenbud-Wigner time delay for Hamiltonians H satisfying Assumption 4.1 with $\mu \geq 5$.

Theorem 4.7. *Let $f \geq 0$ satisfy Assumption 2.1, and let H satisfy Assumption 4.1 with $\mu \geq 5$. Then one has for each $\varphi \in \mathcal{D}_3$ the identity*

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = -i \int_{\mathbb{R}} dx |\varphi(x)|^2 \overline{S(x)} S'(x).$$

Proof. Let $\varphi \in \mathcal{D}_3$. Then $S\varphi \in \mathcal{D}_3$ by Lemma 4.5, and conditions (3.7)-(3.8) are verified by Lemma 4.6. Therefore all the hypotheses of Theorem 3.4 and Remark 3.6 are satisfied, and so the claim is proved. \square

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Appendix

We collect in this appendix some facts on the restriction operator $\gamma(\tau)$ of Lemma 4.4. We consider the general case with configurations space \mathbb{R}^d , $d \geq 1$.

Let $P \equiv (P_1, P_2, \dots, P_d)$ be the vector momentum operator in $L^2(\mathbb{R}^d)$. For each $s \in \mathbb{R}$, we denote by $\mathcal{H}^s(\mathbb{R}^d)$ the completion of the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ on \mathbb{R}^d for the norm $\|\varphi\|_{\mathcal{H}^s(\mathbb{R}^d)} := \|\langle P \rangle^s \varphi\|$. Given $\tau \in \mathbb{R}$, we let $\gamma(\tau) : \mathcal{S}(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^{d-1})$ be the restriction operator defined by $\gamma(\tau)\varphi := \varphi(\tau, \cdot)$. We know from [23, Thm. 2.4.2] that $\gamma(\tau)$ extends uniquely to an element of $\mathcal{B}(\mathcal{H}^s(\mathbb{R}^d), L^2(\mathbb{R}^{d-1}))$ for each $s > 1/2$.

Furthermore $\gamma(\tau)$ is Hölder continuous in τ with respect to the operator norm, namely for each $\tau, \tau' \in \mathbb{R}$ there exists a constant C such that

$$\|\gamma(\tau) - \gamma(\tau')\|_{\mathcal{B}(\mathcal{H}^s(\mathbb{R}^d), \mathcal{L}^2(\mathbb{R}^{d-1}))} \leq C \begin{cases} |\tau - \tau'|^{s-1/2} & \text{if } s \in (\frac{1}{2}, \frac{3}{2}), \\ |\tau - \tau'| \cdot |\ln |\tau - \tau'||| & \text{if } s = \frac{3}{2} \text{ and } |\tau - \tau'| < \frac{1}{2}, \\ |\tau - \tau'| & \text{if } s > \frac{3}{2}. \end{cases} \quad (4.22)$$

Finally $\gamma(\tau)$ has the following differentiability property.

Lemma 4.8. *Let $s > k + \frac{1}{2}$ with $k \geq 0$ integer. Then γ is k times (Hölder continuously) differentiable as a map from \mathbb{R} to $\mathcal{B}(\mathcal{H}^s(\mathbb{R}^d), \mathcal{L}^2(\mathbb{R}^{d-1}))$.*

Proof. We adapt the proof of [20, Lemma 3.3]. Consider first $s > k + \frac{1}{2}$ with $k = 1$. The obvious guess for the derivative at τ of γ is $(D\gamma)(\tau) := \gamma(\tau)\partial_1$, where ∂_1 stands for the partial derivative w.r.t. the first variable. Thus one has for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $\delta \in \mathbb{R}$ with $|\delta| \in (0, 1/2)$

$$\left\{ \frac{1}{\delta} [\gamma(\tau + \delta) - \gamma(\tau)] - (D\gamma)(\tau) \right\} \varphi = \frac{1}{\delta} \int_0^\delta d\xi [(\partial_1 \varphi)(\tau + \xi, \cdot) - (\partial_1 \varphi)(\tau, \cdot)].$$

In particular, using the first (and thus the most pessimistic) bound in (4.22), we get

$$\begin{aligned} & \left\| \left\{ \frac{1}{\delta} [\gamma(\tau + \delta) - \gamma(\tau)] - (D\gamma)(\tau) \right\} \varphi \right\|_{\mathcal{L}^2(\mathbb{R}^{d-1})} \\ & \leq \frac{1}{|\delta|} \int_0^{|\delta|} d\xi \left\| (\partial_1 \varphi)(\tau + \operatorname{sgn}(\delta)\xi, \cdot) - (\partial_1 \varphi)(\tau, \cdot) \right\|_{\mathcal{L}^2(\mathbb{R}^{d-1})} \\ & \leq \|\partial_1 \varphi\|_{\mathcal{H}^{s-1}(\mathbb{R}^d)} \frac{1}{|\delta|} \int_0^{|\delta|} d\xi \|\gamma(\tau + \operatorname{sgn}(\delta)\xi) - \gamma(\tau)\|_{\mathcal{B}(\mathcal{H}^{s-1}(\mathbb{R}^d), \mathcal{L}^2(\mathbb{R}^{d-1}))} \\ & \leq \operatorname{Const.} \|\varphi\|_{\mathcal{H}^s(\mathbb{R}^d)} \frac{1}{|\delta|} \int_0^{|\delta|} d\xi |\xi|^{s-3/2} \\ & \leq \operatorname{Const.} \|\varphi\|_{\mathcal{H}^s(\mathbb{R}^d)} |\delta|^{s-3/2}. \end{aligned}$$

Since $\mathcal{S}(\mathbb{R}^d)$ is dense in $\mathcal{H}^s(\mathbb{R}^d)$ and $D\gamma : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H}^s(\mathbb{R}^d), \mathcal{L}^2(\mathbb{R}^{d-1}))$ is Hölder continuous, the result is proved for $k = 1$. The result for $k > 1$ follows then easily by using the expression for $(D\gamma)(\tau)$. \square

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